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On the Convergence of Local Approximations to Pseudodifferential Operators With Applications

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**ON THE CONVERGENCE OF LOCAL APPROXIMATIONS TO
PSEUDODIFFERENTIAL OPERATORS WITH APPLICATIONS ***

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Abstract. We consider the approximation of a class pseudodifferential operators by sequences of operators which can be expressed as compositions of differential operators and their inverses. We show that the error in such approximations can be bounded in terms of the L_1 error in approximating a convolution kernel, and use this fact to develop convergence results. Our main result is a finite time convergence analysis of the Engquist-Majda [7] Padé approximants to the square root of the d'Alembertian. We also show that no spatially local approximation to this operator can be convergent uniformly in time. We propose some temporally local but spatially nonlocal operators with better long time behavior. These are based on Laguerre and exponential series.

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1. Introduction. Pseudodifferential operators in time and/or space arise naturally in the formulation of many wave propagation problems. Prime examples include the restriction of unbounded domains via the introduction of artificial boundaries [7], the reduction of scattering problems to boundary integral equations [13], the factorization of wave operators into “one-way” equations [2], and the modeling of systems with memory [14]. Although there have been advances in recent years in the efficient application of certain integral operators, a typical approach to the numerical approximation of these problems is to replace the pseudodifferential operator by a combination of differential operators and their inverses, which can then be applied using standard numerical techniques. This is the approach discussed in all the works cited above.

In this note we examine the convergence of sequences of local approximations to a class of pseudodifferential operators. Our main example is the square root of the d’Alembertian, which is important in the study of acoustic, elastic and electromagnetic waves. Although many approximations to this operator have been proposed (e.g. [19]), error estimates of the type considered here do not seem to have been derived. (For estimates based on high-frequency asymptotics see [12].) Our estimates are important if the use of high order conditions is considered, as in [5]. We express the operator as the sum of a differential operator and a convolution operator with an L_1 kernel. Decomposing the local approximation in the same way, we estimate the error in terms of the difference between the exact and approximate convolution kernels. We see that a sequence of local approximations is convergent if its sequence of approximate kernels converges (in L_1) to the exact kernel.

The main result we obtain in this framework is a finite time convergence theorem for the Padé approximants to the square root of the d’Alembertian which were proposed by Engquist and Majda [7]. We also show that this approximation (or any other which is local in space as well as time) is *not* convergent in our sense for infinite time. We propose some new approximations for infinite time which are spatially nonlocal. They are based on Laguerre and exponential series. Although we have not proven convergence for these, we do show that the error is reasonably small uniformly in time. The practical implementation and testing of long-time approximations will be carried out elsewhere.

2. A Class of Pseudodifferential Operators and Local Approximations. We consider first an operator, $\mathcal{A}$, acting on functions of $t \in [0, \infty)$ which vanish along with their derivatives at $t = 0$. We assume:

ASSUMPTION 1.

$$\mathcal{A}u = \sum_{j=0}^p a_j \frac{d^j u}{dt^j} + A_{-1} * u, \quad A_{-1} \in L_1([0, \infty)).$$

Making a Laplace transformation we then obtain:

$$(2.0.1) \quad \hat{\mathcal{A}}(s) = \sum_{j=0}^p a_j s^j + a_{-1}(s),$$

where $a_{-1}(s)$ is the Laplace transform of the function $A_{-1}(t)$. Typically, we know $\hat{\mathcal{A}}$ directly. To verify that Assumption 1 holds we must check that the inverse transform of a_{-1} is in L_1 . Necessary and sufficient conditions for this to hold are given in [20, Ch. 7].

We give two examples, the first of which is relevant to problems involving the wave equation and the second of which is relevant to problems involving the diffusion equation.

Example: Let

$$(2.0.2) \quad \hat{A}(s) = \sqrt{s^2 + 1} = s + \frac{1}{s + \sqrt{s^2 + 1}}.$$

Then [15]

$$(2.0.3) \quad \mathcal{A}u = \frac{du}{dt} + \mathcal{S} * u, \quad \mathcal{S}(t) = \frac{J_1(t)}{t},$$

where $J_1(t)$ is a first order Bessel function. It is easily verified that $\mathcal{S} \in L_1([0, \infty))$ so Assumption 1 holds.

Example: Let

$$(2.0.4) \quad \hat{A}(s) = \sqrt{s + 1}.$$

Then $\mathcal{A}$ does *not* satisfy Assumption 1.

We remark that the second example might be studied by expressing $\mathcal{A}$ as the composition of a differential operator and a convolution. For example,

$$(2.0.5) \quad \sqrt{s + 1} = \frac{1}{\sqrt{s + 1}}(s + 1),$$

implies

$$(2.0.6) \quad \mathcal{A}u = \mathcal{G} * \left(\frac{du}{dt} + u \right), \quad \mathcal{G}(t) = \frac{e^{-t}}{\sqrt{\pi t}}.$$

2.1. Local Approximations. We now consider local approximations $\mathcal{B}$ to operators $\mathcal{A}$ satisfying Assumption 1:

$$(2.1.7) \quad \mathcal{B}u = \sum_{j=0}^p a_j \frac{d^j u}{dt^j} + B_{-1} * u,$$

where we assume that the differential operators in our standard decomposition of $\mathcal{A}$ and $\mathcal{B}$ agree. So that $\mathcal{B}$ will be local, we restrict $B_{-1}(t)$ to the class $\mathcal{R}$ defined by:

DEFINITION 1. A function f is in class $\mathcal{R}$ if its Laplace transform, $\hat{f}(s)$, is a rational function.

Alternatively, $\mathcal{R}$ may be described through the following elementary result. (See [15].)

LEMMA 2.1. The class $\mathcal{R}$ consists of functions which are products of polynomials, exponential functions and trigonometric functions.

The error in approximating $\mathcal{A}$ by $\mathcal{B}$ is equivalent to the error in approximating convolution by A_{-1} by convolution by B_{-1} . We therefore have:

THEOREM 1. Let $u \in L_p([0, T])$, $0 < T \leq \infty$. Then

$$\|(\mathcal{A} - \mathcal{B})u\|_{L_p([0, T])} \leq \|A_{-1} - B_{-1}\|_{L_1([0, T])} \|u\|_{L_p([0, T])}.$$

Proof: Clearly

$$(2.1.8) \quad \|(A - B)u\|_{L_p([0, T])} = \|(A_{-1} - B_{-1}) * u\|_{L_p([0, T])}.$$

The result then follows from the basic inequality $\|f * g\|_{L_p} \leq \|f\|_{L_1} \|g\|_{L_p}$. $\diamond$

By this result we see that the problem of constructing accurate/convergent local approximations is equivalent to approximating the L_1 function A_{-1} by elements of $\mathcal{R}$. We therefore have:

COROLLARY 1. *Let $0 < T \leq \infty$. For any $\epsilon > 0$ there exists a local operator B such that:*

$$\|A - B\|_{L_p([0, T])} < \epsilon.$$

(Here we use the operator norm.)

Proof: We need only show that $\mathcal{R}$ is dense in L_1 . For finite T this follows from the density of the polynomials. For $T = \infty$ we can use the density of certain exponential families, which follows from logarithmic mappings of $[0, \infty)$ to finite intervals. $\diamond$

In subsequent sections we will study the error for specific sequences of approximations. It is nonetheless interesting to consider the possibility of optimal approximations where the degree of the transform of B_{-1} is fixed. For finite intervals and the more restricted class of functions defined by products of polynomials and exponentials, the existence of best approximations in L_1 has been established [4, Ch. 6]. Moreover, for monotone kernels interpolants can be computed and the degree of approximation estimated. In [10], boundary conditions based on time interpolation of $J_1(t)/t$ were proposed and shown to have good L_1 approximation properties.

2.2. Operators in Higher Dimension. In most applications the operators to be approximated act on functions defined on the product of a time interval with a spatial region, Ω . In the simplest case we take Ω to be a hyperplane or torus and assume that $\hat{A}$ is a homogeneous function of s and $|k| = (\sum_j k_j^2)^{1/2}$, where the k_j 's are Fourier variables. For example, if $\hat{A} \equiv \square^{1/2}$ is the square root of the d'Alembertian we have:

$$(2.2.9) \quad \widehat{\square^{1/2}} = \sqrt{s^2 + |k|^2} = s + \frac{|k|}{z + \sqrt{z^2 + 1}}, \quad z = \frac{s}{|k|}.$$

The $|k|$ -dependence of the operator complicates the approximation in a number of ways. First of all, an approximation is local in space only if the coefficients of the rational transform involve only even powers of $|k|$. In the example above, the rational function of z whose inverse transform approximates S must have numerator and denominator of definite and opposite parity in order to be spatially local.

Second, since $|k|$ is not bounded, the approximations must be estimated uniformly in $|k|$. It is even possible that approximations can lead to ill-posed problems for some applications. In [18] the well-posedness of local approximations to the square root of the d'Alembertian is thoroughly studied. For general (spatially nonlocal) approximations such complete results are unknown, but various special cases have been considered [6, 11].

3. The Engquist-Majda Padé Approximants. The best known and most used rational approximations to $\sqrt{s^2 + 1}$ are the Padé approximants suggested by Engquist and Majda [7]. In our language they may be written as (see [19]):

$$(3.0.10) \quad \frac{1}{s + \sqrt{1 + s^2}} \approx i \frac{U_{n-1}(is)}{U_n(is)} = i \frac{\sin n\theta}{\sin(n+1)\theta}, \quad \cos \theta = is,$$

where U_n denotes the Chebyshev polynomial of the second kind. Here we give a completely different derivation of this approximation. We begin with the formula [1, Ch. 9]:

$$(3.0.11) \quad S \equiv \frac{J_1(t)}{t} = \frac{1}{\pi} \int_{-1}^1 \sqrt{1 - w^2} \cos wt \, dw.$$

For fixed t we approximate the integral by the Gaussian quadrature rule appropriate for the weight $\sqrt{1 - w^2}$, based on second kind Chebyshev polynomials [1, Ch. 25]:

$$(3.0.12) \quad \frac{J_1(t)}{t} \approx \mathcal{K}_n(t) \equiv \frac{1}{n+1} \sum_{l=1}^n \sin^2 \left(\frac{l\pi}{n+1} \right) \cos \left(\left(\cos \frac{l\pi}{n+1} \right) t \right) + \frac{\pi}{(2n!)2^{2n+1}} t^{2n} \cos \xi t, \quad -1 < \xi < 1.$$

Laplace transformation in time leads to the formula:

$$(3.0.13) \quad \frac{1}{s + \sqrt{s^2 + 1}} \approx \frac{1}{n+1} \sum_{l=1}^n \sin^2 \left(\frac{l\pi}{n+1} \right) \frac{s}{s^2 + \cos^2 \frac{l\pi}{n+1}}.$$

Remarkably we have:

THEOREM 2. *Approximations (3.0.10) and (3.0.13) are the same.*

Proof: We first note that both expressions represent rational functions with denominators of exact degree n and the same poles, $s = i \cos \frac{l\pi}{n+1}$, $l = 1 \dots n$. Moreover, the numerators are of degree $n-1$. To prove their equality we will multiply each expression by $(s - i \cos \frac{j\pi}{n+1})$ and take the limit $s \rightarrow i \cos \frac{j\pi}{n+1}$. For (3.0.10) this yields:

$$(3.0.14) \quad \frac{(-1)^{j+1}}{n+1} \sin \frac{nj\pi}{n+1} \sin \frac{j\pi}{n+1} = \frac{\sin^2 \frac{j\pi}{n+1}}{n+1}.$$

For (3.0.13) we note that $\cos \frac{j\pi}{n+1} = -\cos \frac{(n+1-j)\pi}{n+1}$. Therefore, the limit process eliminates all but two terms in the sum:

$$(3.0.15) \quad \frac{1}{n+1} \left(\frac{1}{2} \sin^2 \frac{j\pi}{n+1} \pm \frac{1}{2} \sin^2 \frac{(n+1-j)\pi}{n+1} \right).$$

Expressions (3.0.14) and (3.0.15) are clearly equal. This, combined with the fact that the numerators have degree $n-1$, implies that the two functions are the same. $\diamond$

Using the error formula for Gaussian quadrature we directly obtain an error estimate for the approximation, $\mathcal{K}_n(t)$, to $S(t)$:

THEOREM 3. For $0 \leq T < \infty$:

$$\|S - K_n\|_{L_1([0,T])} \leq \min \left(\pi \left(\frac{T}{2} \right)^{2n+1} \frac{1}{(2n+1)!}, \frac{1}{2}T + \|S\|_{L_1([0,\infty))} \right).$$

Proof: Noting that:

$$(3.0.16) \quad |K_n(t)| \leq \frac{1}{n+1} \sum_{l=1}^n \sin^2 \frac{l\pi}{n+1} = \frac{1}{\pi} \int_{-1}^1 \sqrt{1-w^2} dw = \frac{1}{2},$$

we have:

$$(3.0.17) \quad |(J_1(t)/t) - K_n(t)| \leq \min \left(\frac{\pi}{2} \left(\frac{t}{2} \right)^{2n} \frac{1}{(2n)!}, \frac{1}{2} + |(J_1(t)/t)| \right).$$

Integrating this expression yields the desired result. $\diamond$ We note that this result clearly implies the rapid convergence of the approximation for fixed T as n is increased.

This result can be extended to approximation of the pseudodifferential operator $\square^{1/2}$ in higher space dimensions. Introduce the spaces $L_2(H_p, [0, T])$ with norm:

$$(3.0.18) \quad \|u\|_{p,[0,T]}^2 \equiv \int_0^T \int_{R^N} (1 + |k|^2)^p |\hat{u}(k, t)|^2 dk dt.$$

Writing:

$$(3.0.19) \quad \square^{1/2} = \frac{\partial}{\partial t} + \hat{S}(|k|, t), \quad B_n = \frac{\partial}{\partial t} + \hat{K}_n(|k|, t),$$

we have:

THEOREM 4. For any $\epsilon, \delta > 0$, $0 \leq T < \infty$, there exists N such that for any $n > N$ and $u \in L_2(H_p, [0, T])$:

$$\|(\square^{1/2} - B_n)u\|_{p-2-\delta,[0,T]} \leq \epsilon \|u\|_{p,[0,T]}.$$

Proof: We first estimate the error in Fourier space. Note that:

$$(3.0.20) \quad \hat{S}(k, t) = |k|^2 \frac{J_1(|k|t)}{|k|t}, \quad \hat{K}_n(k, t) = \frac{|k|^2}{n+1} \sum_{l=1}^n \sin^2 \frac{l\pi}{n+1} \cos \left(\left(\cos \frac{l\pi}{n+1} \right) |k|t \right).$$

Then:

$$(3.0.21) \quad \|(\hat{S} - \hat{K}_n) * \hat{u}\|_{L_2([0,T])} \leq \|\hat{S} - \hat{K}_n\|_{L_1([0,T])} \|\hat{u}\|_{L_2([0,T])}.$$

The first term on the right can be estimated using the result of Theorem 3 and making the change of variables $z = |k|t$:

$$(3.0.22) \quad \begin{aligned} \|\hat{S} - \hat{K}_n\|_{L_1([0,T])} &= |k| \int_0^{|k|T} \left| (J_1(z)/z) - \frac{1}{n+1} \sum_{l=1}^n \sin^2 \frac{l\pi}{n+1} \cos \left(\left(\cos \frac{l\pi}{n+1} \right) z \right) \right| dz \\ &\leq \min \left(\pi |k| \left(\frac{|k|T}{2} \right)^{2n+1} \frac{1}{(2n+1)!}, \frac{1}{2} |k|^2 T + |k| \| (J_1(\cdot)/(\cdot)) \|_{L_1([0,\infty))} \right). \end{aligned}$$

Given $\epsilon, \delta > 0$ we can clearly choose n sufficiently large that:

$$(3.0.23) \quad (1 + |k|^2)^{-(1+(\delta/2))} \|\hat{S} - \hat{K}_n\|_{L_1([0,T])} \leq \epsilon.$$

Finally:

$$(3.0.24) \quad \begin{aligned} \|\mathcal{S} - \mathcal{K}_n\|_{p-2-\delta, [0,T]}^2 &\leq \int_{\mathbb{R}^N} (1 + |k|^2)^p (1 + |k|^2)^{-(2+\delta)} \|\hat{S} - \hat{K}_n\|_{L_1([0,T])}^2 \|\hat{u}\|_{L_2([0,t])}^2 dk \\ &\leq \epsilon^2 \|u\|_{p, [0,T]}^2, \end{aligned}$$

completing the proof. $\diamond$

We are confident that this convergence result can be translated into a convergence result for the artificial boundary problem for smooth solutions of the wave equation in simple domains, using for example the stability results of Ha-Duong and Joly [9]. This, along with some numerical experiments, will be the subject of future work.

4. Long Time Approximations. The error estimates discussed above are strongly dependent on T and break down as $T \rightarrow \infty$. For some applications, for example the so-called limiting amplitude problem [6, 11], or applications to viscoelasticity [14], long time approximations are desired. Also, such approximations will have better large $|k|$ behavior for multidimensional problems. To achieve this we must approximate the convolution kernel in $L_1([0, \infty))$ by functions in our class $\mathcal{R}$. This greatly constrains the functions at our disposal as seen in the following elementary result:

THEOREM 5. *A function $r \in \mathcal{R}$ is an element of $L_1([0, \infty))$ if and only if all poles of $\hat{r}$ lie in the left half complex plane.*

Proof: Simply note that the only functions in $\mathcal{R}$ which are in $L_1([0, \infty))$ take the form of (sums of) polynomials multiplying exponentials where the exponent has negative real part. The transform of such a function has a pole in the left half plane. $\diamond$

An immediate corollary of this result is:

COROLLARY 2. *A function $r \in \mathcal{R} \cap L_1([0, \infty))$ cannot have a transform which may be written as the ratio of polynomials of definite parity.*

For the multidimensional operator associated with $\sqrt{s^2 + |k|^2}$, our corollary implies that long time approximate conditions, in the sense described here, cannot be local in space. For the half-space problem they generally involve the operator whose symbol is $|k|$. This is the so-called Dirichlet-to-Neumann map for the Laplace equation in the half space. The use of this operator for long time solutions of the wave equation has been suggested in [6] and [11]. A key practical issue is the efficient application of the nonlocal map. For progress in this regard see [8, 16].

4.1. Laguerre Expansions. The kernels we wish to approximate, in particular $\mathcal{S}(t)$, are generally in $L_2([0, \infty))$. In L_2 , convergent approximating sequences are easily constructed via expansions in orthogonal functions. A complete set of orthogonal functions whose elements are in $\mathcal{R}$ are the Laguerre functions:

$$(4.1.25) \quad \mathcal{L}_n(\gamma t) = e^{-\frac{\gamma}{2} t} L_n(\gamma t), \quad \hat{\mathcal{L}}_n = \frac{(s - \frac{\gamma}{2})^n}{(s + \frac{\gamma}{2})^{n+1}}.$$

m	g_m	$\ \sum g_m \mathcal{L}_m - \mathcal{S}\ _{L_1([0,\infty))}$	$\ \sum g_m \mathcal{L}_m - \mathcal{S}\ _{L_2([0,\infty))}$
0	0.75	0.87	0.22
1	-0.15	0.79	0.19
2	-0.186	0.60	0.11
3	1.992×10^{-2}	0.59	0.11
4	9.4512×10^{-2}	0.48	7.2×10^{-2}
5	2.08554×10^{-2}	0.48	7.0×10^{-2}
6	-4.94016×10^{-2}	0.42	5.7×10^{-2}
7	-3.34492×10^{-2}	0.41	5.0×10^{-2}
8	1.96034×10^{-2}	0.38	4.7×10^{-2}
9	3.24971×10^{-2}	0.35	3.9×10^{-2}
10	3.04379×10^{-4}	0.35	3.9×10^{-2}

TABLE 1

Coefficients and L_p errors for Laguerre approximations to $\mathcal{S}$, $\gamma = 3/2$.

Here, $L_n(z)$ is the n th Laguerre polynomial and $\gamma > 0$ is a parameter which may be chosen to optimize the convergence rate. The expansion of a kernel $\mathcal{G}$ is given by:

$$(4.1.26) \quad \mathcal{G} \approx \sum_{n=0}^m g_n \mathcal{L}_n(\gamma t), \quad g_n = \gamma \int_0^\infty \mathcal{L}_n(\gamma t) \mathcal{G}(t) dt.$$

We have written a program in Maple to compute these coefficients for arbitrary γ and the kernel $J_1(t)/t$. We have numerically computed the L_1 errors in the resulting approximations. We find $\gamma = 3/2$ to be a convenient choice, both from the point of view of convergence of the series and simplicity of expansion coefficients. The results are given in Table 1. For reference we note that the L_1 norm of $\mathcal{S}$ is about 1.6 and the L_2 norm is about .65.

It is evident that the convergence rate of this series in L_1 is slow at best. Indeed, Laguerre series are *not* generally convergent in L_1 . (See [17].) We do not even have a proof in this particular case. We have not yet implemented boundary conditions based on these expansions, but plan to do so in the future.

4.2. Exponential Expansions. Another convenient set of orthogonal functions in $\mathcal{R}$ are exponential polynomials:

$$(4.2.27) \quad \mathcal{P}_n(\gamma t) = e^{-\frac{\gamma t}{2}} P_n(2e^{-\gamma t} - 1),$$

where $P_n(z)$ is the n th Legendre polynomial and $\gamma > 0$ is again a free parameter. The orthogonality of these functions is easily established by mapping $[0, \infty)$ to $[-1, 1]$ by $z = 2e^{-\gamma t} - 1$. We then expand a kernel $\mathcal{G}$ by:

$$(4.2.28) \quad \mathcal{G} \approx \sum_{n=0}^m g_n \mathcal{P}_n(\gamma t), \quad g_n = \gamma(2n+1) \int_0^\infty \mathcal{P}_n(\gamma t) \mathcal{G}(t) dt.$$

The Laplace transform of $\mathcal{P}_n$ takes the form:

$$(4.2.29) \quad \hat{\mathcal{P}}_n = \sum_{j=0}^n \frac{a_{nj}}{s + \frac{(2j+1)\gamma}{2}},$$

m	g_m	$\ \sum g_m \mathcal{P}_m - \mathcal{S}\ _{L_1([0,\infty))}$	$\ \sum g_m \mathcal{P}_m - \mathcal{S}\ _{L_2([0,\infty))}$
0	1.80998×10^{-1}	2.1	0.51
1	3.49884×10^{-1}	1.2	0.24
2	1.49008×10^{-1}	0.81	0.19
3	-1.46339×10^{-1}	0.76	0.14
4	-1.24158×10^{-1}	0.59	0.10
5	9.35578×10^{-2}	0.52	8.1×10^{-2}
6	4.84350×10^{-2}	0.50	7.5×10^{-2}
7	-8.60302×10^{-2}	0.43	5.7×10^{-2}
8	2.89748×10^{-2}	0.41	5.4×10^{-2}
9	3.50595×10^{-2}	0.41	5.1×10^{-2}
10	-5.67689×10^{-2}	0.38	4.3×10^{-2}

TABLE 2

Coefficients and L_p errors for exponential Legendre approximations to $\mathcal{S}$, $\gamma = 1/5$.

where the coefficients a_{nj} are easily tabulated. We have written a Maple procedure to compute the expansion coefficients for $\mathcal{S}$, and have tabulated the results in Table 2. We found that $\gamma = 1/5$ was a reasonable choice from the point of view of speed of convergence.

Again the convergence of the series is rather slow, particularly in L_1 , and the errors are generally larger than for the corresponding term in the Laguerre series. Moreover, we have no convergence proof.

4.3. Other Approximations. Given the disappointing convergence behavior of the series above, we are led to consider other means for constructing long time approximations. One possibility is to consider the integral representation of $\mathcal{S}$ used in our analysis of the Padé approximants (3.0.11). Setting $z = i\omega$ and rewriting it as a contour integral along the imaginary axis, we can then deform the contour into the left half plane. A quadrature scheme will then produce approximations which decay exponentially in t . We plan to investigate this procedure in future work.

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